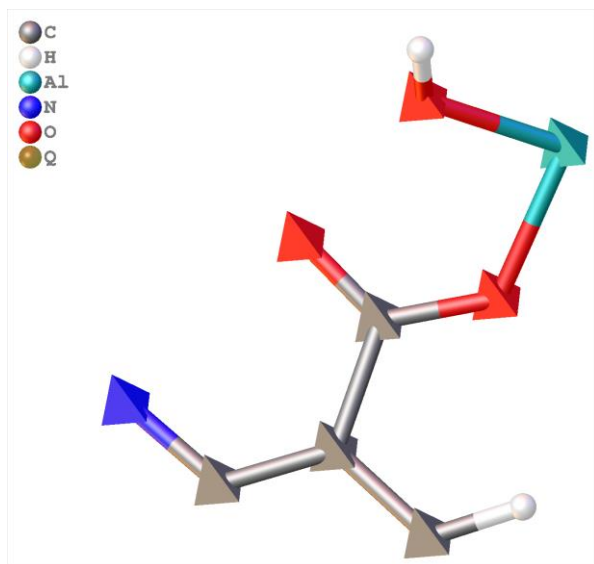


$R_1 = 19.25\%$

Crystal Data and Experimental



Crystal Data. CHNOAl, $M_r = 70.01$, monoclinic, $I2/a$ (No. 15), $a = 6.553(2)$ Å, $b = 7.480(3)$ Å, $c = 18.995(6)$ Å, $\beta = 93.74(4)^\circ$, $\alpha = \gamma = 90^\circ$, $V = 929.1(6)$ Å³, $T = 175.00(10)$ K, $Z = 1$, $Z' = 0.125$, $\mu(\text{electron}) = 0.000$, 2224 reflections measured, 800 unique ($R_{\text{int}} = 0.1790$) which were used in all calculations. The final wR_2 was 0.5159 (all data) and R_1 was 0.1925 ($I > 2(I)$).

Compound	exp_7301
Formula	CHNOAl
$D_{calc.}/\text{g cm}^{-3}$	0.125
μ/mm^{-1}	0.000
Formula Weight	70.01
Colour	None None None
Shape	?
Size/ mm^3	? \times ? \times ?
T/K	175.00(10)
Crystal System	monoclinic
Space Group	$I2/a$
$a/\text{\AA}$	6.553(2)
$b/\text{\AA}$	7.480(3)
$c/\text{\AA}$	18.995(6)
$\alpha/^\circ$	90
$\beta/^\circ$	93.74(4)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	929.1(6)
Z	1
Z'	0.125
Wavelength/ \AA	0.0251
Radiation type	electron
$\Theta_{min}/^\circ$	0.076
$\Theta_{max}/^\circ$	0.898
Measured Refl.	2224
Independent Refl.	800
Reflections with $I > 2(I)$	307
R_{int}	0.1790
Parameters	80
Restraints	214
Largest Peak	0.305
Deepest Hole	-0.336
GooF	2.052
wR_2 (all data)	0.5159
wR_2	0.4151
R_1 (all data)	0.3023
R_1	0.1925

Structure Quality Indicators

Reflections:	d min (0.0251) 2 Θ =1.8°	0.80	I/ σ (I)	5.0	Rint m=2.91	17.90%	Full 1.7°	83.9
	Shift	-0.603	Max Peak	0.3	Min Peak	-0.3	Goof	2.052

Experimental Extended. A None None None ? -shaped crystal with dimensions ? ×? ×? mm³ was mounted on a suitable support. Data were collected using an XtaLAB Synergy-ED, HyPix-ED, electron source at 200keV diffractometer operating at $T = 175.00(10)$ K.

Data were measured using continuous rotation electron diffraction of 0.2° per frame for 0.2 s using electron radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro (Rigaku) The maximum resolution that was achieved was $\Theta = 0.898^\circ$ (0.80 Å).

The diffraction pattern was indexed The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro (Rigaku) and the unit cell was refined using CrysAlisPro (Rigaku, V1.171.44.70a, 2024) on 500 reflections, 22% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro (Rigaku, V1.171.44.70a, 2024). The final completeness is 83.90 % out to 0.898° in Θ . No absorption correction was performed. The absorption coefficient μ of this material is 0.000 mm⁻¹ at this wavelength ($\lambda = 0.025\text{\AA}$) and the minimum and maximum transmissions are 0 and 0.

The structure was solved and the space group $I2/a$ (# 15) determined by the ShelXT 2018/2 (Sheldrick, 2018) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of ShelXL 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Most hydrogen atom positions were calculated geometrically and refined using the riding model, but some hydrogen atoms were refined freely.

Table 1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **exp_7301**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	x	y	z	U_{eq}
Al00	5000	5000	5000	29.1(16)
C002	2700(30)	3260(20)	6026(6)	29.1(16)
O003	1110(20)	3220(15)	5630(5)	29.1(16)
O004	4510(20)	3699(17)	5822(5)	29.2(16)
O005	2500	6120(30)	5000	28.9(16)
C006	4340(30)	3166(18)	7243(6)	29.1(16)
C007	2470(30)	2800(20)	6788(7)	29.1(16)
C008	740(30)	2084(19)	7030(6)	29.2(16)
N1	-1080(40)	1860(30)	6628(10)	29.2(16)

Table 2: Anisotropic Displacement Parameters ($\times 10^4$) **exp_7301**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \dots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al00	48(3)	39(3)	-0.6(18)	0.4(6)	-5(2)	-0.2(6)
C002	48(3)	39(3)	-0.6(17)	0.6(6)	-4.6(19)	-0.2(6)
O003	48(3)	39(3)	-0.6(17)	0.6(6)	-4.5(19)	-0.2(6)
O004	48(3)	39(3)	-0.6(17)	0.6(6)	-4.5(19)	-0.1(6)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O005	48(3)	39(3)	-1.5(18)	0	-5(2)	0
C006	48(3)	39(3)	-0.6(17)	0.7(7)	-5(2)	-0.2(7)
C007	48(3)	39(3)	-0.6(17)	0.7(7)	-5(2)	-0.2(7)
C008	48(3)	39(3)	-0.6(17)	0.7(7)	-5(2)	-0.2(7)
N1	48(3)	39(3)	-0.6(18)	0.6(7)	-5(2)	-0.3(7)

Table 3: Bond Lengths in Å for **exp_7301**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Al00	O003 ¹	1.904(10)	C002	C007	1.505(18)
Al00	O003 ²	1.904(10)	C006	C007	1.476(19)
Al00	O004 ³	1.885(11)	C006	C008 ⁴	1.397(16)
Al00	O004	1.885(11)	C007	C008	1.36(2)
Al00	O005	1.840(9)	C008	N1	1.38(3)
Al00	O005 ³	1.840(9)	----		
C002	O003	1.242(17)			¹ 1/2+x,1-y,+z; ² 1/2-x,+y,1-z; ³ 1-x,1-y,1-z;
C002	O004	1.32(2)			⁴ 1/2-x,1/2-y,3/2-z

Table 4: Bond Angles in ° for **exp_7301**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O003 ¹	Al00	O003 ²	180.0	O003	C002	C007	116.5(16)
O004 ³	Al00	O003 ²	94.7(5)	O004	C002	C007	119.2(11)
O004	Al00	O003 ¹	94.7(5)	C002	O003	Al00 ¹	129.5(11)
O004	Al00	O003 ²	85.3(5)	C002	O004	Al00	125.3(9)
O004 ³	Al00	O003 ¹	85.3(5)	Al00 ¹	O005	Al00	125.8(11)
O004	Al00	O004 ³	180.0(8)	C008 ⁴	C006	C007	118.3(17)
O005 ³	Al00	O003 ¹	89.2(6)	C006	C007	C002	113.0(15)
O005	Al00	O003 ²	89.2(6)	C008	C007	C002	123.5(12)
O005	Al00	O003 ¹	90.8(6)	C008	C007	C006	123.5(12)
O005 ³	Al00	O003 ²	90.8(6)	C007	C008	C006 ⁴	118.0(13)
O005 ³	Al00	O004 ³	92.1(5)	C007	C008	N1	124.7(14)
O005 ³	Al00	O004	87.9(5)	N1	C008	C006 ⁴	116.5(19)
O005	Al00	O004	92.1(5)	----			
O005	Al00	O004 ³	87.9(5)				¹ 1/2-x,+y,1-z; ² 1/2+x,1-y,+z; ³ 1-x,1-y,1-z;
O005	Al00	O005 ³	180.0				⁴ 1/2-x,1/2-y,3/2-z
O003	C002	O004	124.3(12)				

Table 5: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **exp_7301**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	x	y	z	U_{eq}
H006	5723.68	3618.1	7019.77	35
H005	2200(110)	7350(40)	4850(30)	27(18)

Table 6: Atomic Occupancies for all atoms that are not fully occupied in **exp_7301**.

Atom	Occupancy
N1	0.5

Citations

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.